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Coulombic interactions and multicomponent ionic dispersion during transport of charged species in heterogeneous porous media

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ABSTRACT

Electrochemical cross-coupling plays a significant role for transport of charged species in porous media [1, 2]. In this study we performed flow-through experiments in a quasi two-dimensional setup using dilute solutions of strong electrolytes to study the influence of charge interactions on mass transfer of ionic species in saturated porous media. The experiments were carried out under advection-dominated conditions (seepage velocity: 1 and 1.5 m/day) in two well-defined heterogeneous domains where flow diverging around a low-permeability inclusion and flow focusing in high-permeability zones occurred. To quantitatively interpret the outcomes of our laboratory experiments in the spatially variable flow fields we developed a two dimensional numerical model based on a multicomponent formulation, on charge conservation and on the accurate description of transverse dispersion. The results of the multicomponent transport simulations were compared with the high-resolution (5 mm spacing) concentration measurements of the ionic species at the outlet of the flow-through domain. The excellent agreement between the measured concentrations and the results of purely forward numerical simulations demonstrates the capability of the proposed two-dimensional multicomponent approach to describe transport of charged species and to accurately capture the Coulombic interactions between the ions, which are clearly observed in the flow-through experiments. Furthermore, the model allowed us to directly quantify and visualize the ionic interactions by mapping the Coulombic cross-coupling between the dispersive fluxes of the charged species in the heterogeneous domains.

The outcomes of this study are important in many subsurface applications including migration of contaminants and propagation of reaction fronts.

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